

AD-A230 179

REPORT DOCUMENTATION PAGE

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1. AGENCY USE ONLY (Leave blank) 2. REPORT DATE December 27, 1990 3. REPORT TYPE AND DATES COVERED FINAL - May 1, 1988 - September 30, 1990

4. TITLE AND SUBTITLE
ADAPTIVE COMPUTATIONS FOR PARTIAL DIFFERENTIAL EQUATIONS GOVERNING ADVECTIVE FLUID FLOWS

5. FUNDING NUMBERS
N00 14-88-K-0370
(WYOM 5/3313)

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8. PERFORMING ORGANIZATION REPORT NUMBER

N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
University of Wyoming
Contracts and Grants Accounting
P.O. Box 3355
Laramie, WY 82071

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

N/A

11. SUPPLEMENTARY NOTES (Abstract continued from Block 13 below) (applying conjugate-gradient and conjugate-residual methods to solve the large, sparse linear systems arising from the discretization of the governing equations), and the exploitation of parallel and vector computer architectures.

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Unclassified/Unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words) We developed improved approaches to the numerical simulation of highly advective fluid flows using adaptive computational schemes. (Applications include heat and mass transfer in flowing fluids, reaction-diffusion phenomena of combustion, bubbly and multiphase flows, underwater explosions, and electrochemistry). Solutions to the equations governing these flows commonly exhibit highly localized features -- steep moving fronts, moving boundaries, unstable interfaces -- not captured by standard numerical techniques with acceptable accuracy and computational cost. We developed adaptive techniques in which computational degrees of freedom are allocated according to qualitative properties of the equations being solved, to efficiently enhance local resolution.

We focused on adaptive gridding methods (implementing adaptive local gridding algorithms, in which a code automatically refines the finite-element or finite-difference grid in zones needing temporarily increased numerical resolution), front-tracking algorithms (generalizing a sophisticated front-tracking code first developed for strictly hyperbolic systems of conservation laws, based on the numerical tracking of an interface via sequences of Riemann problems), development of efficient iterative schemes and preconditioners for large linear systems (continued in Block 11 above)

14. SUBJECT TERMS

adaptive grid refinement techniques, multiphase flow, conjugate gradient methods, front-tracking methods, convection-diffusion equations

15. NUMBER OF PAGES

11

16. PRICE CODE

N/A

17. SECURITY CLASSIFICATION OF REPORT

Unclassified

18. SECURITY CLASSIFICATION OF THIS PAGE

Unclassified

19. SECURITY CLASSIFICATION OF ABSTRACT

Unclassified

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OFFICE OF NAVAL RESEARCH
FINAL REPORT
for
1 MAY 1988 THROUGH 30 SEPTEMBER 1990
CONTRACT No. 0014-88-K-0370

ADAPTIVE COMPUTATIONS FOR
PARTIAL DIFFERENTIAL EQUATIONS
GOVERNING ADVECTIVE FLUID FLOWS

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December 1990

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BRIEF SUMMARY OF RESEARCH

Task 1. Properties of Differential Equation Models

In [18,32,40] we studied stability properties of unstable fluid flow. We presented the effects of the nonlinearities and properties such as bifurcation in [18,36,51]. Stability of multiphase flow was studied in [32]. This gives us insight into the important properties of unstable, bubbly flow.

Special properties and treatment of singularities in the solutions to partial differential equations were presented in [4,39]. Asymptotic behavior of solutions was studied in [12,36]. Properties of hyperbolic conservation laws and non-hyperbolic systems were analyzed in [17,18,36,37,39,52]. Properties of models of various types were considered in [4,62,63].

Finally, unknown parameters must often be determined in various partial differential equation models. Special direct marching methods to treat unknown coefficients in time-dependent problems have been developed in [31,38,65-68,76].

Task 2. Analysis of Numerical Procedures

Numerical properties of the various discretization schemes for the partial differential equation models must also be well understood. Stability and accuracy for finite element methods are studied in [2,6,7,30,35,41,56,70,74], for finite strip methods in [19-21], and for collocation methods in [14,53,54]. Analysis for models for chemically reacting flows is presented in [8,15,35,42,72,75].

Accuracy of fluid velocities is essential in the coupled systems in our models. Mixed finite element methods have been studied in [30,34,42,45]. Mixed methods have been coupled with other techniques in multicomponent and multiphase problems in [16,36,40,50,64,81,84,87]. The degeneracies in the multiphase case cause difficulties in the analysis [16].

Hyperbolic, near hyperbolic, and non-hyperbolic systems were studied in [2,5,33], in connection with convection-diffusion-like problems in [5,54]. Front tracking methods have been analyzed via Riemann problems in [36,39,52]. Hyperbolic equations are also used in inverse methods for seismic prospecting, sonar, nondestructive testing, etc. Extensive work on accuracy of numerical methods for interface conditions was studied in [25,79,89].

Operator splitting techniques [2,3,16,72,81,86] have been presented using modified method of characteristics concepts [2,8,16,43,73,84]. When applied to multiphase problems or problems with nonlinear flux functions, the operator splitting methods also utilize Petrov-Galerkin methods [2,41,73] when the problems are not fully symmetrized by the modified method of characteristics. Extensions of these methods to Eulerian-Lagrangian Localized Adjoint Methods (ELLAM) conserve mass and treat boundary conditions well [29,51,77,86,88].

Full asymptotic error estimates are developed for the difficult coupled systems of partial differential equations in [6,13,42,45]. Superconvergence results for mixed finite element methods along Gauss lines were obtained in [34].

Flow of various fluids through heterogeneous media can be quite unstable, with fingering instabilities. Development of effective parameters to model those instabilities for nonlinear scale-up is considered in [32,78,80,82].

Task 3. Adaptive Local Grid Refinement

A major effort has been concentrated on various aspects of adaptive local grid refinement. Elementwise local refinement techniques were presented in [7,53] for Burgers' Equation. Adaptive techniques that entail error estimators or AI strategies were discussed in [1,7,10,16,48,53].

Purely local refinement techniques which involve data structure trees have been described in [1,10,33]. A more efficient method that requires a simpler data structure is a "patch refinement" technique [3,40,44,46,48,65,71,82]. Aspects of accuracy of the composite grid were considered in [22,23,46,57,61,65] and efficiency of solution in [24,44,46,87]. BEPS and FAC methods are presented and compared in [9,22,28,46,57,65]. Extensions of these concepts to local time-stepping methods appear in [27,60]. Applications of these methods in industrial-level simulators appeared in [22-24].

The application of patch method to follow and resolve moving fluid interfaces is presented in [16,41]. Parallel aspects appeared in [14,55].

Several aspects of front tracking methods have been studied. Riemann problem analyses appeared in [36,39,52] while the complications due to non-hyperbolic systems were studied in [18,39,52]. Combinations with mixed finite element methods are considered in [34,45,47].

Task 4. Computational Considerations

The advent of parallel and vector computer architectures and visualization capabilities are revolutionizing computational considerations. Basic efficiency considerations were discussed in [3,10,47,49,59]. Parallel and vector techniques have been presented in [1,14,19,21,46,55,83], with scheduling analysis in [1]. Many of the local grid refinement techniques have been based upon domain decomposition methods [3,9,12,16,28,41,44,50,80]. The potential for parallelization of the modified method of characteristics was pointed out in several papers and is currently being implemented.

Due to the size and poor conditioning of the systems involved, preconditioned iterative methods are essential for linear solution. Preconditioners are presented for conjugate gradients, conjugate residuals, and domain decomposition methods in [3,9,44,85].

Finally, we have made substantial progress in visualization on our Ardent Titan and our Silicon Graphics workstation. This greatly aids our computational capabilities, allowing us to use the computers in an experimental mode to build intuition.

We emphasize that the combination of modeling, analysis, numerical analysis, and computing skills is essential in addressing the complex and unstable coupled systems of partial differential equations used to model problems of interest to the Navy.

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